



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:48 am BST

PDB ID : 3AV6
Title : Crystal structure of mouse DNA methyltransferase 1 with AdoMet
Authors : Takeshita, K.; Suetake, I.; Yamashita, E.; Suga, M.; Narita, H.; Nakagawa, A.; Tajima, S.
Deposited on : 2011-02-22
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

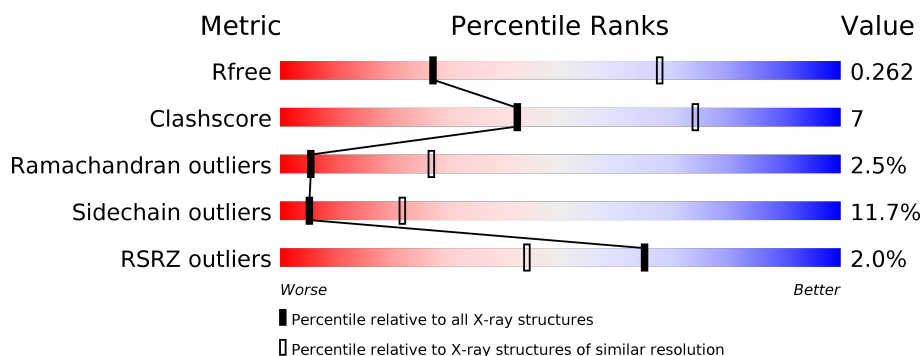
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1330	<div> <div>2%</div> <div>62%</div> <div>21%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9110 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

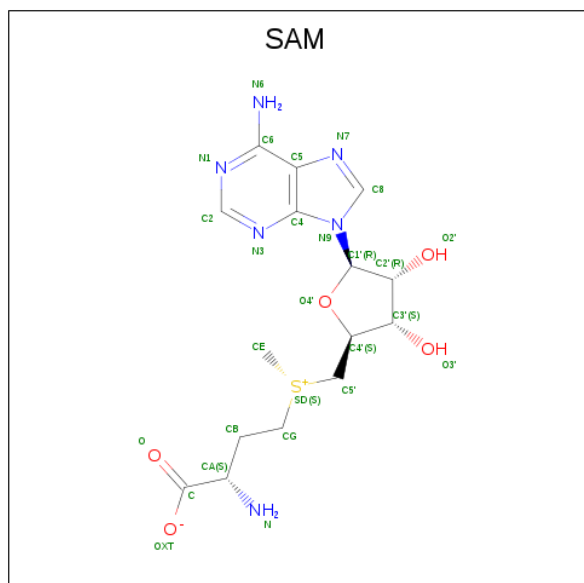
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1135	Total	C	N	O	S	0	0	0
			9079	5744	1579	1697	59			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

H1543	W1439	Q1306
H1544	R1440	T1312
E1545		R1313
Q1546	Q1446	R1314
V1549	V1447	I1317
R1553	R1448	
	L1449	A1320
R1557	G1450	F1330
	D1451	P1333
	G1452	V1336
H1575	A1455	F1337
R1576	L1458	V1346
Q1577	Q1459	V1354
A1587		S1355
S1601	F1462	N1356
	H1463	R1359
A1603	D1464	L1360
ALA	L1475	S1361
VAL		S1362
LYS	V1478	R1366
LYS	C1479	V1370
GLU	S1480	R1371
GLU	C1481	
ALA	A1482	M1374
ALA		S1385
THR	D1488	E1394
LYS	P1489	P1395
	E1490	L1403
ASP	S1491	H1407
	R1492	Y1408
	W1500	Q1409
		P1410
	H1504	I1411
	N1507	L1412
	R1508	R1413
	A1513	T1416
	Y1516	C1417
	D1522	K1418
	F1525	D1419
	T1528	M1420
	V1529	A1426
	T1530	H1430
	N1531	
	P1532	
	K1537	
	V1541	
	L1542	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.00Å 97.14Å 130.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.14 – 3.09 43.14 – 3.09	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.14-3.09) 99.6 (43.14-3.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.02 (at 3.12Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.8.0	Depositor
R, R_{free}	0.191 , 0.255 0.198 , 0.262	Depositor DCC
R_{free} test set	1626 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9110	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SAM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/9299	0.79	2/12573 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1360	LEU	C-N-CA	7.21	139.73	121.70
1	A	1042	ILE	C-N-CA	6.25	137.34	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9079	0	8847	124	0
2	A	4	0	0	0	0
3	A	27	0	22	0	0
All	All	9110	0	8869	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1543:HIS:HD2	1:A:1546:GLN:H	1.21	0.88
1:A:885:LYS:HA	1:A:886:THR:HG23	1.60	0.82
1:A:975:GLU:OE1	1:A:978:ARG:HD2	1.81	0.80
1:A:886:THR:H	1:A:887:GLN:HG2	1.50	0.77
1:A:1543:HIS:CD2	1:A:1546:GLN:H	2.02	0.76
1:A:1488:ASP:O	1:A:1491:SER:HB3	1.88	0.73
1:A:1159:HIS:HE1	1:A:1166:THR:H	1.37	0.72
1:A:1543:HIS:CD2	1:A:1545:GLU:H	2.10	0.70
1:A:1043:ASN:ND2	1:A:1085:ARG:O	2.23	0.66
1:A:1541:VAL:HG13	1:A:1549:VAL:HG22	1.78	0.65
1:A:1234:GLY:HA3	1:A:1278:ARG:HH21	1.62	0.63
1:A:783:THR:HG21	1:A:897:CYS:HB2	1.80	0.63
1:A:1023:LYS:O	1:A:1048:SER:HB3	1.99	0.62
1:A:753:VAL:HG22	1:A:761:GLU:HB3	1.81	0.62
1:A:1333:PRO:HD2	1:A:1359:ARG:HB2	1.82	0.61
1:A:1478:VAL:HG13	1:A:1500:TRP:NE1	2.17	0.60
1:A:445:ALA:O	1:A:458:GLY:HA3	2.02	0.59
1:A:1157:GLY:HA3	1:A:1587:ALA:HB3	1.85	0.58
1:A:929:SER:HB3	1:A:938:ARG:HG2	1.83	0.58
1:A:992:PRO:HD2	1:A:1336:VAL:HG22	1.86	0.58
1:A:1543:HIS:HD2	1:A:1545:GLU:H	1.53	0.57
1:A:1530:THR:O	1:A:1575:HIS:HB3	2.05	0.56
1:A:1229:CYS:O	1:A:1231:GLY:N	2.38	0.56
1:A:1413:ARG:O	1:A:1553:ARG:HD2	2.05	0.56
1:A:1374:MET:HE1	1:A:1525:PHE:HZ	1.70	0.56
1:A:1023:LYS:HE2	1:A:1052:ALA:HB2	1.87	0.54
1:A:522:LEU:HD11	1:A:587:MET:HE3	1.88	0.54
1:A:472:LEU:H	1:A:603:ALA:HB1	1.73	0.54
1:A:1139:LEU:HD21	1:A:1163:ILE:HG22	1.89	0.53
1:A:526:PRO:O	1:A:527:ASP:HB2	2.09	0.53
1:A:595:GLY:HA3	1:A:1504:HIS:CE1	2.44	0.53
1:A:380:ALA:HB1	1:A:462:LYS:HB3	1.90	0.53
1:A:955:LYS:NZ	1:A:955:LYS:H	2.07	0.53
1:A:1330:PHE:H	1:A:1356:ASN:HD21	1.57	0.52
1:A:1005:CYS:HB2	1:A:1017:ILE:HA	1.90	0.52
1:A:1385:SER:C	1:A:1416:ILE:HD11	2.30	0.52
1:A:1371:ARG:NH2	1:A:1522:ASP:OD1	2.44	0.51
1:A:774:SER:O	1:A:776:PRO:HD3	2.10	0.51
1:A:1171:GLU:O	1:A:1191:THR:HA	2.10	0.50
1:A:386:MET:HG3	1:A:459:ILE:HD13	1.93	0.50
1:A:1306:GLN:HB3	1:A:1333:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:THR:CG2	1:A:1366:ARG:HH22	2.24	0.50
1:A:410:MET:HG2	1:A:491:GLU:HB2	1.93	0.50
1:A:535:ASN:O	1:A:539:THR:HB	2.12	0.50
1:A:1407:HIS:HD2	1:A:1409:GLN:HE21	1.60	0.49
1:A:580:PRO:HD2	1:A:583:LEU:HD12	1.94	0.49
1:A:1143:ARG:HG2	1:A:1167:LEU:HD11	1.94	0.49
1:A:1449:LEU:HD21	1:A:1455:ALA:HB2	1.94	0.49
1:A:730:ASN:HD21	1:A:732:ASP:HB2	1.77	0.49
1:A:770:PRO:HB3	1:A:778:TYR:CE1	2.47	0.49
1:A:886:THR:OG1	1:A:887:GLN:HA	2.13	0.49
1:A:705:ASP:O	1:A:1235:MET:HB2	2.12	0.48
1:A:567:VAL:HG13	1:A:581:ILE:HG23	1.95	0.48
1:A:793:MET:HB3	1:A:828:LEU:HD12	1.95	0.48
1:A:1030:THR:HG22	1:A:1032:ARG:H	1.78	0.48
1:A:966:ASP:HB2	1:A:967:PRO:HD2	1.96	0.47
1:A:1275:VAL:HG22	1:A:1283:LEU:HD22	1.95	0.47
1:A:376:HIS:CE1	1:A:462:LYS:HB2	2.50	0.47
1:A:1027:PRO:O	1:A:1030:THR:HB	2.14	0.47
1:A:1370:VAL:O	1:A:1374:MET:HG2	2.15	0.47
1:A:1254:PHE:HD2	1:A:1268:LEU:HD12	1.80	0.46
1:A:1002:GLU:HB2	1:A:1020:ARG:HB3	1.98	0.46
1:A:1302:LEU:O	1:A:1314:ARG:HA	2.16	0.46
1:A:783:THR:CG2	1:A:897:CYS:HB2	2.45	0.46
1:A:1274:PHE:HA	1:A:1277:TYR:CD1	2.51	0.46
1:A:522:LEU:HB3	1:A:581:ILE:HG13	1.97	0.46
1:A:1462:PHE:O	1:A:1475:LEU:HB3	2.16	0.45
1:A:639:ILE:HD11	1:A:1238:PHE:HB3	1.97	0.45
1:A:1302:LEU:HD12	1:A:1317:ILE:HD13	1.98	0.45
1:A:1374:MET:HE1	1:A:1525:PHE:CZ	2.50	0.45
1:A:1275:VAL:HG11	1:A:1346:VAL:HG22	1.99	0.45
1:A:1440:ARG:NH2	1:A:1513:ALA:HA	2.31	0.45
1:A:357:PRO:HB2	1:A:366:LEU:HD22	1.98	0.45
1:A:1403:LEU:HD12	1:A:1557:ARG:HD3	1.99	0.45
1:A:414:THR:HG22	1:A:415:SER:H	1.82	0.45
1:A:472:LEU:H	1:A:603:ALA:CB	2.29	0.45
1:A:1266:PHE:HB3	1:A:1320:ALA:HB3	1.98	0.45
1:A:978:ARG:NH2	1:A:1507:ASN:OD1	2.50	0.45
1:A:392:LEU:HB3	1:A:411:HIS:CE1	2.52	0.45
1:A:780:ALA:HB2	1:A:799:TRP:CE3	2.51	0.45
1:A:533:LEU:HD22	1:A:537:ILE:HD12	1.98	0.44
1:A:513:TYR:CE2	1:A:517:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:LEU:HB2	1:A:753:VAL:HG12	1.99	0.44
1:A:914:VAL:HA	1:A:930:ILE:HG22	2.00	0.44
1:A:472:LEU:HD21	1:A:512:ILE:HG12	2.00	0.44
1:A:1464:ASP:HA	1:A:1482:ALA:HB1	1.98	0.44
1:A:735:SER:HA	1:A:793:MET:HE1	1.98	0.44
1:A:1420:MET:HA	1:A:1420:MET:HE2	2.00	0.44
1:A:1439:TRP:HB3	1:A:1516:TYR:HB2	2.00	0.44
1:A:1426:ALA:O	1:A:1430:HIS:HD2	2.01	0.44
1:A:1360:LEU:CB	1:A:1361:SER:HB2	2.47	0.43
1:A:811:THR:HG21	1:A:1284:LYS:HB3	2.01	0.43
1:A:1048:SER:OG	1:A:1050:GLU:HB2	2.18	0.43
1:A:726:LYS:HA	1:A:770:PRO:HA	2.00	0.43
1:A:371:LEU:HD11	1:A:424:HIS:CD2	2.52	0.43
1:A:776:PRO:O	1:A:777:LEU:HB2	2.19	0.43
1:A:526:PRO:O	1:A:527:ASP:CB	2.67	0.43
1:A:1246:PHE:HA	1:A:1249:SER:HB3	2.02	0.42
1:A:1330:PHE:H	1:A:1356:ASN:ND2	2.17	0.42
1:A:802:ALA:HA	1:A:817:LEU:HD12	2.00	0.42
1:A:964:LYS:O	1:A:965:LYS:HB2	2.20	0.42
1:A:980:TYR:HA	1:A:981:SER:HA	1.73	0.42
1:A:723:GLN:N	1:A:724:GLY:HA3	2.34	0.42
1:A:1143:ARG:HB2	1:A:1221:GLU:HG3	2.01	0.42
1:A:1394:GLU:HG3	1:A:1395:PRO:HD2	2.02	0.41
1:A:1360:LEU:HD22	1:A:1360:LEU:HA	1.89	0.41
1:A:413:PHE:HD2	1:A:416:PHE:HB3	1.85	0.41
1:A:594:ALA:HB1	1:A:1492:ARG:HH21	1.85	0.41
1:A:635:PHE:HD1	1:A:1243:TYR:CD2	2.39	0.41
1:A:1223:LEU:CB	1:A:1263:PRO:HG3	2.50	0.41
1:A:1144:THR:HA	1:A:1222:MET:O	2.20	0.41
1:A:1076:GLN:HE22	1:A:1080:GLN:HG3	1.84	0.41
1:A:1173:TRP:CD1	1:A:1175:PRO:HD2	2.56	0.41
1:A:588:ARG:O	1:A:592:HIS:HD2	2.03	0.41
1:A:955:LYS:HZ2	1:A:955:LYS:H	1.69	0.41
1:A:1418:LYS:HD2	1:A:1532:PRO:HD2	2.03	0.41
1:A:434:GLU:C	1:A:436:ASN:H	2.24	0.41
1:A:1151:CYS:HB3	1:A:1577:GLN:HG2	2.03	0.41
1:A:414:THR:HG21	1:A:453:PRO:O	2.21	0.41
1:A:1030:THR:C	1:A:1032:ARG:H	2.23	0.40
1:A:631:PHE:HE1	1:A:1246:PHE:CE2	2.38	0.40
1:A:381:VAL:O	1:A:461:GLY:HA2	2.22	0.40
1:A:664:GLN:O	1:A:692:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:CYS:HB3	1:A:900:CYS:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1113/1330 (84%)	991 (89%)	94 (8%)	28 (2%)	5	27

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	GLY
1	A	573	ALA
1	A	772	ASP
1	A	777	LEU
1	A	896	PHE
1	A	965	LYS
1	A	1230	GLN
1	A	1233	SER
1	A	1361	SER
1	A	430	THR
1	A	476	ASP
1	A	732	ASP
1	A	1037	SER
1	A	408	SER
1	A	730	ASN
1	A	850	GLY
1	A	1229	CYS
1	A	1513	ALA
1	A	480	LYS
1	A	603	ALA

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Mol	Chain	Res	Type
1	A	921	VAL
1	A	1038	TYR
1	A	379	ASP
1	A	776	PRO
1	A	922	ASP
1	A	1362	SER
1	A	1410	PRO
1	A	409	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1000/1162 (86%)	883 (88%)	117 (12%)	5 22

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	A	385	GLN
1	A	405	TYR
1	A	406	GLU
1	A	408	SER
1	A	410	MET
1	A	414	THR
1	A	421	SER
1	A	429	ASP
1	A	448	ILE
1	A	451	GLU
1	A	459	ILE
1	A	469	GLN
1	A	476	ASP
1	A	479	GLU
1	A	481	VAL
1	A	500	GLU
1	A	507	LEU

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Mol	Chain	Res	Type
1	A	515	SER
1	A	533	LEU
1	A	539	THR
1	A	548	VAL
1	A	549	ASN
1	A	581	ILE
1	A	590	LEU
1	A	602	ARG
1	A	639	ILE
1	A	640	GLU
1	A	654	ARG
1	A	656	CYS
1	A	666	GLU
1	A	693	ARG
1	A	697	LEU
1	A	710	ASP
1	A	719	LYS
1	A	723	GLN
1	A	725	LYS
1	A	727	LYS
1	A	728	LYS
1	A	729	GLN
1	A	749	TYR
1	A	755	ILE
1	A	758	GLU
1	A	759	MET
1	A	772	ASP
1	A	775	LYS
1	A	779	LEU
1	A	817	LEU
1	A	826	MET
1	A	844	GLU
1	A	845	ASN
1	A	865	LYS
1	A	872	TRP
1	A	876	GLU
1	A	882	SER
1	A	892	ASN
1	A	900	CYS
1	A	902	ARG
1	A	915	LEU
1	A	917	GLN

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Mol	Chain	Res	Type
1	A	920	GLU
1	A	943	VAL
1	A	951	THR
1	A	955	LYS
1	A	981	SER
1	A	990	ASP
1	A	1005	CYS
1	A	1008	LYS
1	A	1012	VAL
1	A	1040	THR
1	A	1042	ILE
1	A	1055	ASN
1	A	1062	ARG
1	A	1066	GLU
1	A	1094	SER
1	A	1095	LYS
1	A	1142	LEU
1	A	1197	LEU
1	A	1198	LEU
1	A	1199	LYS
1	A	1207	THR
1	A	1209	SER
1	A	1213	ARG
1	A	1223	LEU
1	A	1229	CYS
1	A	1232	PHE
1	A	1237	ARG
1	A	1241	ARG
1	A	1270	ASN
1	A	1271	VAL
1	A	1272	ARG
1	A	1275	VAL
1	A	1289	CYS
1	A	1292	ARG
1	A	1312	THR
1	A	1313	ARG
1	A	1317	ILE
1	A	1337	PHE
1	A	1354	VAL
1	A	1360	LEU
1	A	1361	SER
1	A	1412	LEU

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Mol	Chain	Res	Type
1	A	1416	ILE
1	A	1446	GLN
1	A	1448	ARG
1	A	1451	ASP
1	A	1458	LEU
1	A	1459	GLN
1	A	1480	SER
1	A	1490	GLU
1	A	1508	ARG
1	A	1528	THR
1	A	1537	LYS
1	A	1541	VAL
1	A	1549	VAL
1	A	1576	ARG
1	A	1601	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	HIS
1	A	468	ASN
1	A	469	GLN
1	A	730	ASN
1	A	892	ASN
1	A	917	GLN
1	A	953	ASN
1	A	1076	GLN
1	A	1159	HIS
1	A	1212	GLN
1	A	1239	ASN
1	A	1402	GLN
1	A	1409	GLN
1	A	1430	HIS
1	A	1446	GLN
1	A	1509	HIS
1	A	1543	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SAM	A	1	-	21,29,29	1.17	0	18,42,42	2.29	6 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAM	A	1	-	-	3/8/33/33	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	SAM	O3'-C3'-C4'	-4.88	96.94	111.05
3	A	1	SAM	N3-C2-N1	-4.04	122.36	128.68
3	A	1	SAM	C5'-SD-CG	3.72	112.90	103.40
3	A	1	SAM	C4-C5-N7	-3.08	106.19	109.40
3	A	1	SAM	O4'-C1'-C2'	-3.05	102.47	106.93
3	A	1	SAM	O2'-C2'-C3'	2.93	121.29	111.82

There are no chirality outliers.

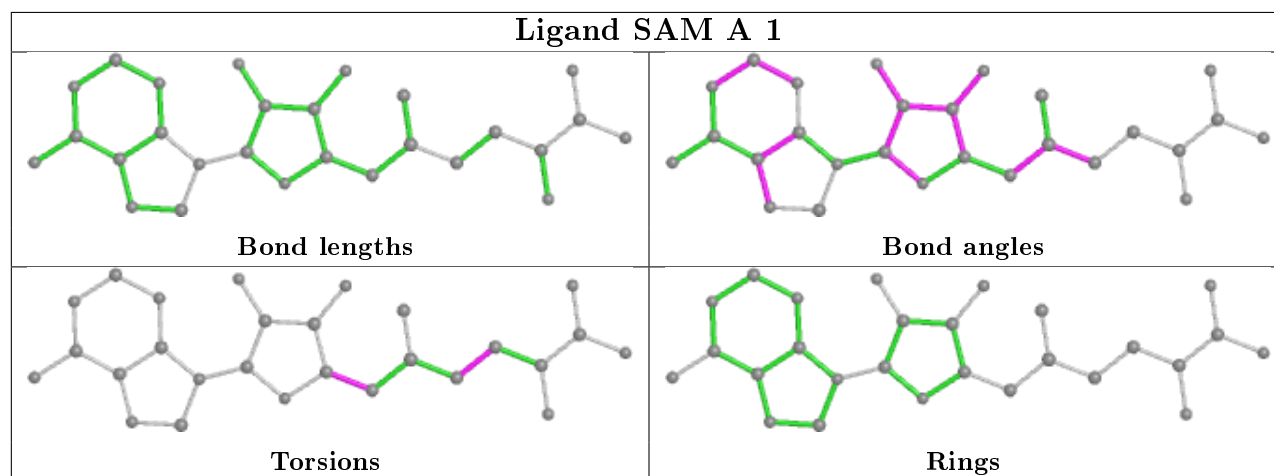
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	SAM	CA-CB-CG-SD
3	A	1	SAM	O4'-C4'-C5'-SD
3	A	1	SAM	C3'-C4'-C5'-SD

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1135/1330 (85%)	-0.13	23 (2%) 65 44	13, 52, 100, 127	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	SER	4.3
1	A	390	GLU	4.2
1	A	923	GLY	3.9
1	A	379	ASP	3.2
1	A	378	GLU	3.1
1	A	405	TYR	3.0
1	A	1001	LYS	2.9
1	A	1022	TYR	2.8
1	A	1452	GLY	2.8
1	A	919	GLU	2.8
1	A	547	ASN	2.6
1	A	654	ARG	2.5
1	A	636	SER	2.4
1	A	409	PRO	2.4
1	A	1240	SER	2.4
1	A	918	ILE	2.4
1	A	1451	ASP	2.3
1	A	653	ARG	2.2
1	A	1007	LYS	2.1
1	A	1006	GLY	2.1
1	A	1450	GLY	2.1
1	A	662	CYS	2.0
1	A	1005	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

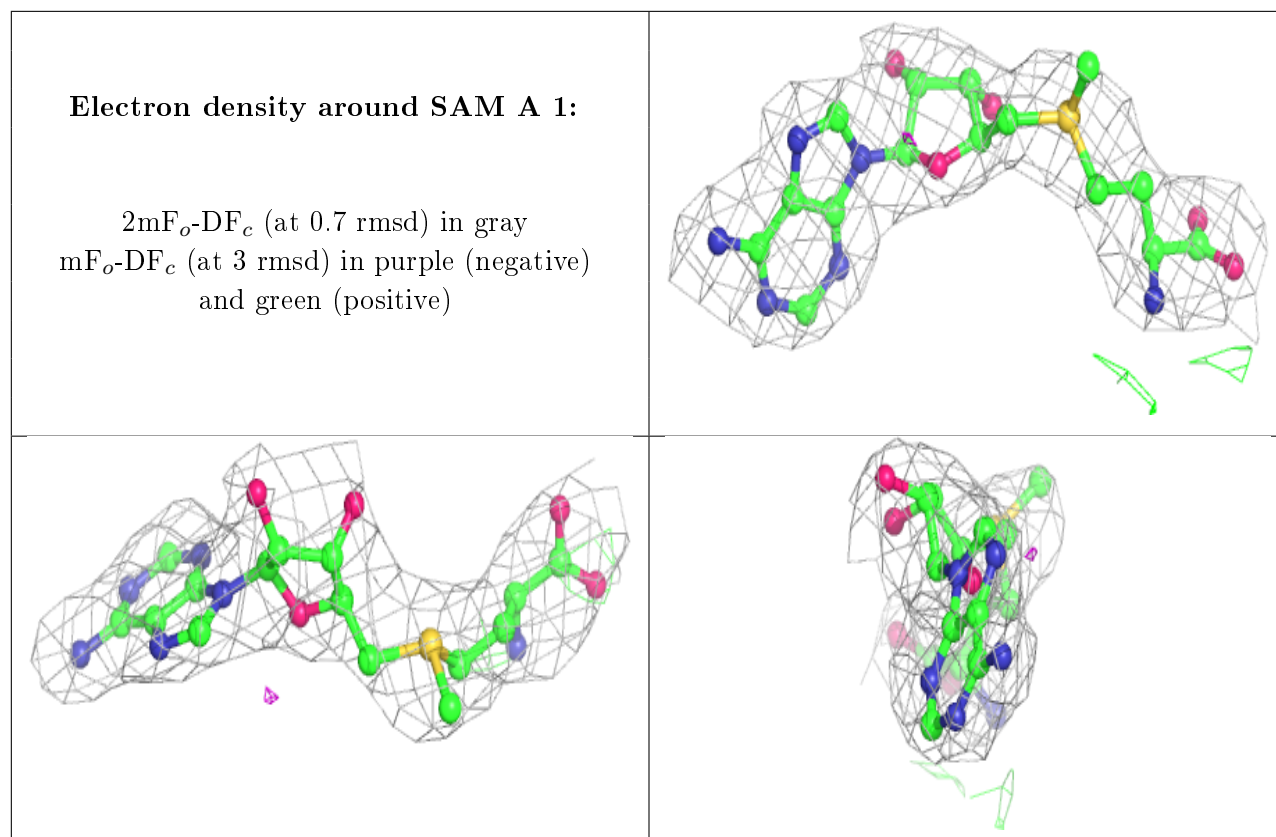
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SAM	A	1	27/27	0.97	0.17	42,43,50,51	0
2	ZN	A	2001	1/1	0.99	0.14	55,55,55,55	0
2	ZN	A	2005	1/1	1.00	0.11	33,33,33,33	0
2	ZN	A	2002	1/1	1.00	0.07	58,58,58,58	0
2	ZN	A	2004	1/1	1.00	0.10	47,47,47,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.